

10/820904

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STRUCTURE FILE UPDATES: 14 MAY 2006 HIGHEST RN 884198-07-6  
DICTIONARY FILE UPDATES: 14 MAY 2006 HIGHEST RN 884198-07-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when  
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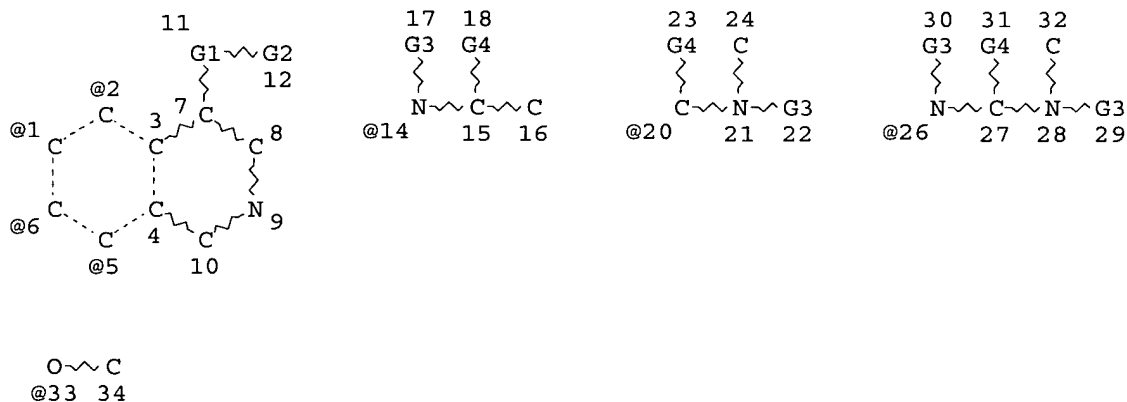
\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

L1 STR



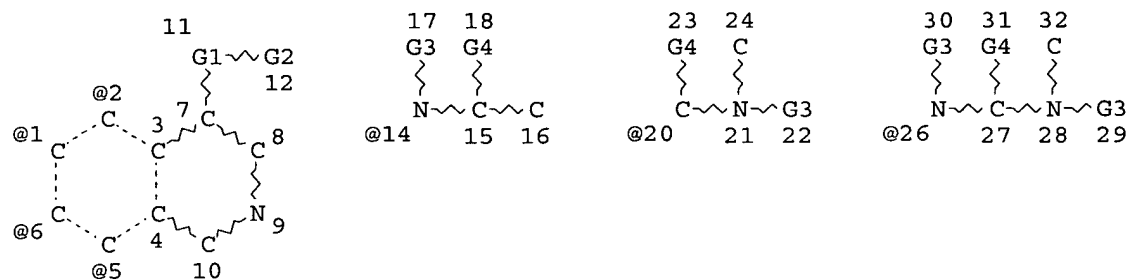
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VAR G3=H/AK  
VAR G4=S/O  
VPA 33-1/2/5/6 U  
NODE ATTRIBUTES:

10/820904

NSPEC IS RC AT 16  
NSPEC IS RC AT 24  
NSPEC IS RC AT 32  
NSPEC IS RC AT 34  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE  
L2 ( 69)SEA FILE=REGISTRY SSS FUL L1  
L3 STR



O~C  
@33 34

REP G1=(1-4) CH2  
VAR G2=14/20/26  
VAR G3=H/AK  
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VPA 33-1/2/5/6 U

NODE ATTRIBUTES:  
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STEREO ATTRIBUTES: NONE  
L4 29 SEA FILE=REGISTRY SUB=L2 SSS FUL L3

100.0% PROCESSED 69 ITERATIONS  
SEARCH TIME: 00.00.01

29 ANSWERS

FILE 'CAPLUS' ENTERED AT 12:23:02 ON 15 MAY 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 15 May 2006 VOL 144 ISS 21  
FILE LAST UPDATED: 14 May 2006 (20060514/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

L5 3 L4

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:837274 CAPLUS

DOCUMENT NUMBER: 141:332067

TITLE: Preparation of isoquinolines as melatonin receptors ligands

INVENTOR(S): Poissonnier-Durieux, Sophie; Wallez, Valerie; Gasnereau, Anne; Yous, Said; Lesieur, Daniel; Delagrang, Philippe; Renard, Pierre; Bennejean, Caroline; Boutin, Jean Albert; Audinot, Valerie

PATENT ASSIGNEE(S): Les Laboratoires Servier, Fr.

SOURCE: Eur. Pat. Appl., 29 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1466604	A1	20041013	EP 2004-290918	20040407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
FR 2853649	A1	20041015	FR 2003-4381	20030409
ZA 2004002657	A	20041014	ZA 2004-2657	20040101
NO 2004001313	A	20041011	NO 2004-1313	20040330
JP 2004307492	A2	20041104	JP 2004-104291	20040331
CA 2462939	AA	20041009	CA 2004-2462939	20040406
CN 1535957	A	20041013	CN 2004-10031034	20040407
BR 2004001031	A	20050118	BR 2004-1031	20040407
US 2004204449	A1	20041014	US 2004-820904	20040408
AU 2004201595	A1	20041028	AU 2004-201595	20040408
NZ 532221	A	20050729	NZ 2004-532221	20040408
PRIORITY APPLN. INFO.:			FR 2003-4381	A 20030409

OTHER SOURCE(S): MARPAT 141:332067

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [wherein Y = (CH<sub>2</sub>)<sub>n</sub>; n = 1-3; A = NR-(C:Z)-R'; NR-(C:Z)-NR'R'', or CZNRR'; Z = S, O; R, R' = independently H, alkyl; R' = alk(en/yn)yl, cycloalkyl, cycloalkylalkyl, hetero/aryl, hetero/arylalkyl; X = N; NR<sub>1</sub>; R<sub>1</sub> = H, cyclo/cycloalkyl/alkyl, hetero/aryl, hetero/aroyl, hetero/arylalkyl; R<sub>2</sub> = cyclo/cycloalkyl/alkyloxy; with provisos; their enantiomers and diastereomers, and their addition salts with a pharmaceutically acceptable acid or base] were prepared as melatonin receptors ligands. Six biol. tests are given. For instance, reacting II•HCl over Pd/C in the presence of TEA/toluene, followed by treatment with MeNH<sub>2</sub>, containing 40% water, gave isoquinoline III. III displayed K<sub>i</sub> values of 9.12•10<sup>-9</sup> M and 2.16•10<sup>-9</sup> M for the binding to MT<sub>1</sub> and MT<sub>2</sub> melatonin receptor in an assay using 2-[125I]-iodomelatonin as radioligand. I acted powerfully on the circadian rhythm via melatoninergetic system (no data). I are useful for treating melatoninergetic system related diseases.

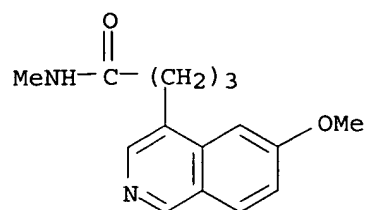
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 773897-21-5P, N-[2-(6-Methoxy-1,2,3,4-tetrahydro-4-isoquinolinyl)ethyl]cyclobutanecarboxamide hydrochloride  
 773897-22-6P, N-[2-(6-Methoxy-4-isoquinolinyl)ethyl]acetamide  
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 773897-25-9P, N-[2-(6-Methoxy-4-isoquinolinyl)ethyl]cyclopropanecarboxamide hydrochloride 773897-26-0P,  
 N-[2-(6-Methoxy-2-phenyl-1,2,3,4-tetrahydro-4-isoquinolinyl)ethyl]acetamide hydrochloride 773897-27-1P,  
 N-[2-(2-Benzyl-6-methoxy-1,2,3,4-tetrahydro-4-isoquinolinyl)ethyl]acetamide 773897-28-2P,  
 N-[2-[2-(3-Formylphenyl)-6-methoxy-1,2,3,4-tetrahydro-4-isoquinolinyl]ethyl]acetamide 773897-29-3P,  
 N-[2-(6-Methoxy-2-methyl-1,2,3,4-tetrahydro-4-isoquinolinyl)ethyl]acetamide hydrochloride 773897-30-6P,  
 N-[2-[2-(Cyclopropylmethyl)-6-methoxy-1,2,3,4-tetrahydro-4-isoquinolinyl]ethyl]acetamide hydrochloride 773897-31-7P,  
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 , N-[2-(6-Methoxy-4-isoquinolinyl)ethyl]propanamide  
 773897-35-1P, N-[2-(6-Methoxy-4-isoquinolinyl)ethyl]cyclopropanecarboxamide 773897-36-2P, N-[2-(6-Methoxy-2-phenyl-1,2,3,4-tetrahydro-4-isoquinolinyl)ethyl]acetamide 773897-37-3P,  
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 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(melatonin receptor ligand; preparation of isoquinolines for treating melatoninergetic system diseases)

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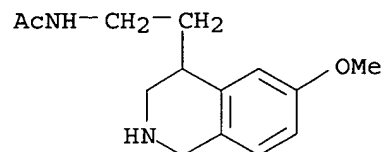
10/820904

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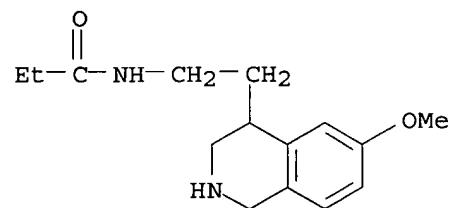
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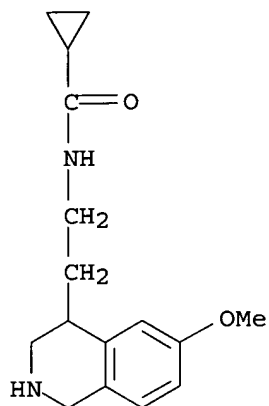


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RN 773897-20-4 CAPLUS

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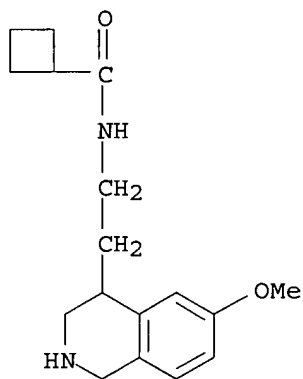
10/820904



● HCl

RN 773897-21-5 CAPLUS

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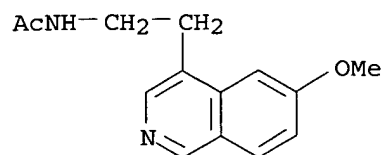


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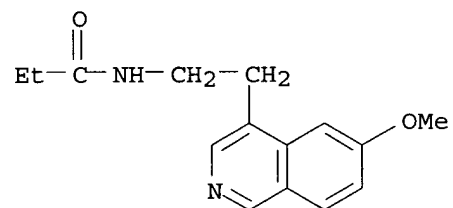
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10/820904



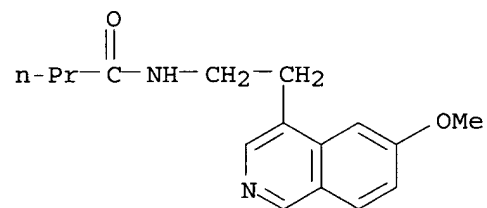
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● HCl

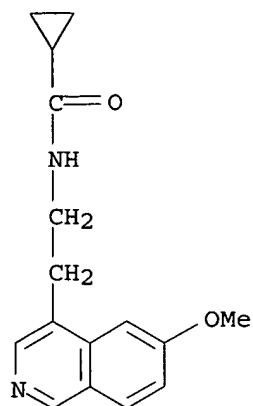
RN 773897-24-8 CAPLUS  
CN Butanamide, N-[2-(6-methoxy-4-isoquinolinylyl)ethyl]-, monohydrochloride  
(9CI) (CA INDEX NAME)



● HCl

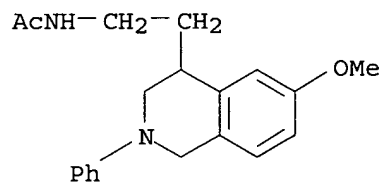
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10/820904



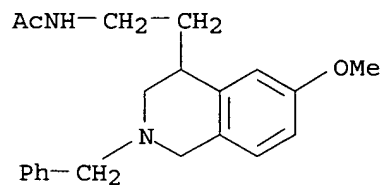
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● HCl

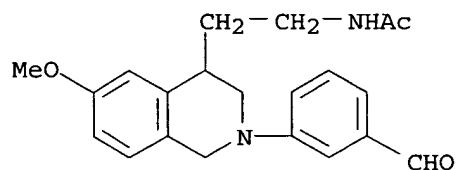
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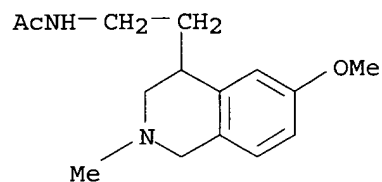
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10/820904

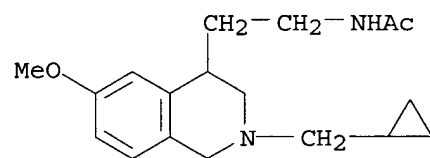


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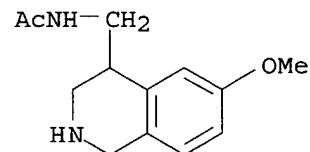
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● HCl

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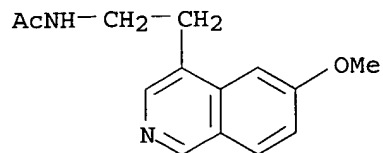


● HCl

10/820904

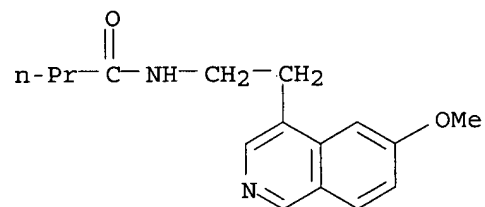
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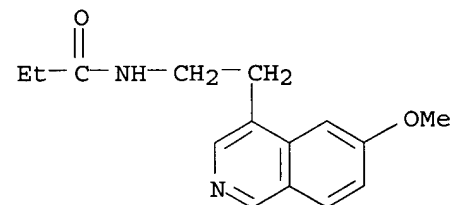
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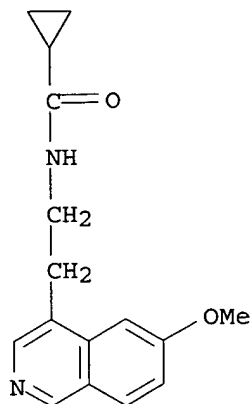
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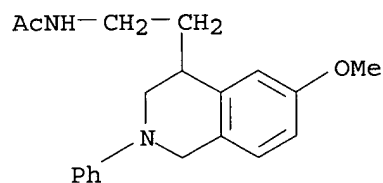
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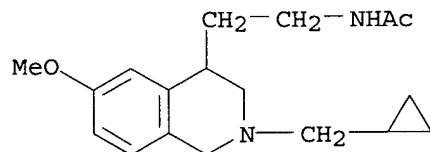
RN 773897-36-2 CAPLUS

CN Acetamide, N-[2-(1,2,3,4-tetrahydro-6-methoxy-2-phenyl-4-isoquinolinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 773897-37-3 CAPLUS

CN Acetamide, N-[2-[2-(cyclopropylmethyl)-1,2,3,4-tetrahydro-6-methoxy-4-isoquinolinyl]ethyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:487577 CAPLUS

DOCUMENT NUMBER: 137:63420

TITLE: Preparation of lactone ketolide macrolide erythromycin antibiotics

INVENTOR(S): Andreotti, Daniele; Arista, Luca; Biondi, Stefano; Cardullo, Francesca; Damiani, Frederica; Lociuero, Sergio; Marchioro, Carla; Merlo, Giancarlo; Mingardi, Anna; Niccolai, Daniela; Paio, Alfredo; Piga, Elisabetta; Pozzan, Alfonso; Seri, Catia; Tarsi, Luca; Terreni, Silvia; Tibasco, Jessica

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 215 pp.

CODEN: PIXXD2

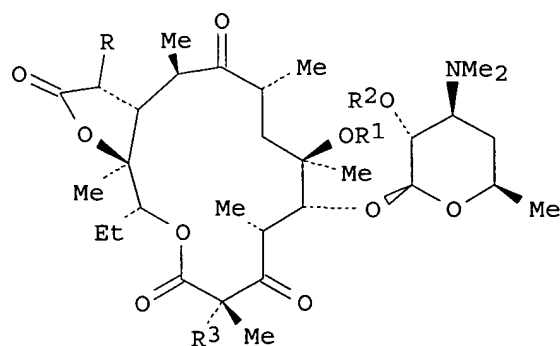
DOCUMENT TYPE: Patent

10/820904

LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002050091	A1	20020627	WO 2001-GB5665	20011220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2432429	AA	20020627	CA 2001-2432429	20011220
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EP 1363925	A1	20031126	EP 2001-271380	20011220
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CN 1492874	A	20040428	CN 2001-822651	20011220
BR 2001016431	A	20040622	BR 2001-16431	20011220
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ZA 2003004748	A	20040423	ZA 2003-4748	20030619
NO 2003002846	A	20030820	NO 2003-2846	20030620
US 2004077557	A1	20040422	US 2003-450893	20031119
US 2005215495	A1	20050929	US 2005-127701	20050512
PRIORITY APPLN. INFO.:			GB 2000-31309	A 20001221
			GB 2001-26276	A 20011101
			GB 2001-26277	A 20011101
			WO 2001-GB5665	W 20011220
			US 2003-450893	B1 20031119

OTHER SOURCE(S): MARPAT 137:63420  
GI



I

AB The present invention relates to lactone ketolides I wherein R is H,

CN, substituted alkyl; R1 is alkyl, alkenyl; R2 is H, hydroxy protecting group; R3 is H, halogen, and pharmaceutically acceptable salts and solvates thereof, to process for their preparation and their use in therapy or prophylaxis of systemic or topical bacterial infections in a human or animal body. Thus, (11S,21R)-3-decladinosyl-11,12-dideoxy-6-O-methyl-3-oxo-12,11-[oxycarbonyl-(cyano)-methylene]erythromycin A was prepared and tested as antibacterial agent against *Streptococcus pneumoniae* and *Streptococcus pyogenes* (MIC  $\leq 1 \mu\text{g/mL}$ ).

IT 439102-96-2P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

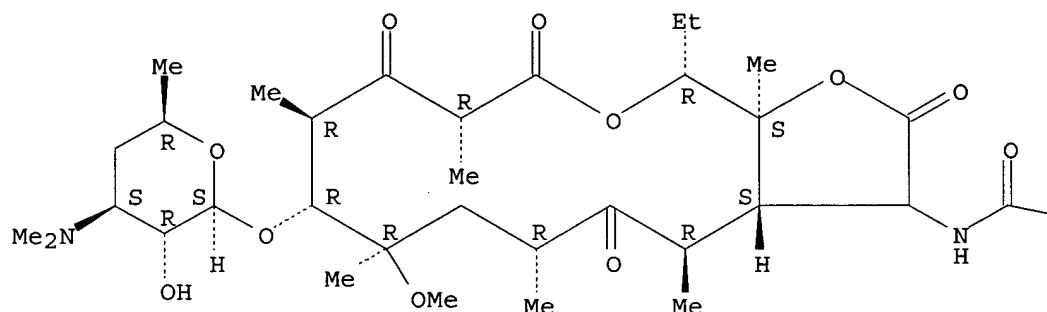
(preparation of lactone ketolide macrolide erythromycin antibiotics and their use in therapy or prophylaxis of systemic or topical bacterial infections)

RN 439102-96-2 CAPLUS

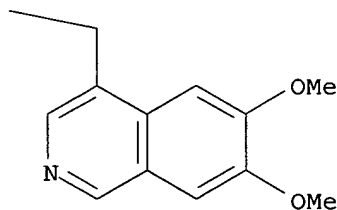
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Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



10/820904

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:23726 CAPLUS

DOCUMENT NUMBER: 110:23726

TITLE: Preparation of heteroaromatic amine derivatives of  
isoindoles and isoquinolines for treatment of  
heart insufficiency and ischemic heart diseases

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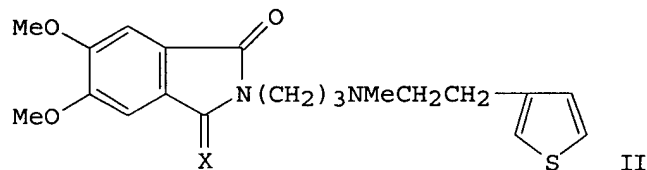
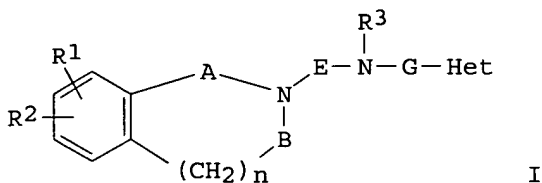
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PATENT INFORMATION:

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EP 269968	A2	19880608	EP 1987-117201	19871121
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R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
DE 3640641	A1	19880714	DE 1986-3640641	19861128
US 4912115	A	19900327	US 1987-125626	19871125
DD 270911	A5	19890816	DD 1987-309530	19871126
IL 84612	A1	19920329	IL 1987-84612	19871126
DK 8706250	A	19880529	DK 1987-6250	19871127
FI 8705233	A	19880529	FI 1987-5233	19871127
NO 8704955	A	19880530	NO 1987-4955	19871127
AU 8781876	A1	19880602	AU 1987-81876	19871127
AU 600995	B2	19900830		
JP 63150276	A2	19880622	JP 1987-299612	19871127
HU 48619	A2	19890628	HU 1987-5359	19871127
HU 206208	B	19920928		
ZA 8708914	A	19890726	ZA 1987-8914	19871127
US 5116986	A	19920526	US 1991-696677	19910507
PRIORITY APPLN. INFO.:			DE 1986-3640641	A 19861128
			US 1989-455722	B1 19891222
			US 1990-627514	B1 19901214

OTHER SOURCE(S): CASREACT 110:23726; MARPAT 110:23726

GI



AB The title compds. [I; A, B = CH<sub>2</sub>, CO, CS; only 1 of A, B may be CS, in which case the other = CH<sub>2</sub>; E = C1-3 alkyl-(un)substituted, linear C2-4 alkylene; G = C1-3 alkyl-(un)substituted, linear C1-6 alkylene; R<sub>1</sub>, R<sub>2</sub> = H, C1-3 alkyl, C1-3 alkoxy; R<sub>1</sub>R<sub>2</sub> = OCH<sub>2</sub>O, OCH<sub>2</sub>CH<sub>2</sub>O; R<sub>3</sub> = H, C1-3 alkyl, phenyl-C1-3 alkyl, C3-5 alkenyl; Het = 5- or 6-membered, N-containing heteroaryl, bonded via N or C, optionally containing O, S, or

an

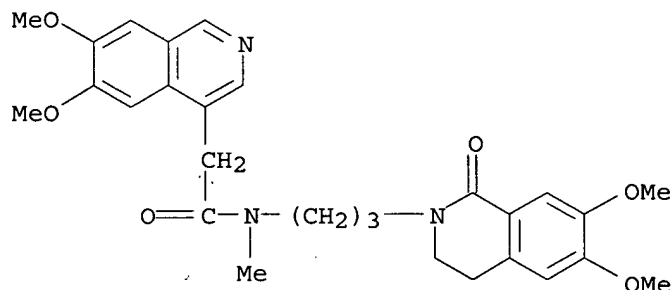
addnl. N, and optionally bearing 1 or 2 substituents or a fused carbocycle; N = 0, 1], their N-oxides, enantiomers, diastereomers, and acid salts were prepared for treatment of heart failure and ischemia. 2-[3-(Methylamino)propyl]phthalimide was N-alkylated with 3-(2-bromoethyl)thiophene to give 44% isoindolinedione II (X = O) which was reduced with Zn powder in HOAc to give, after acidification with aqueous HCl, 70% II·2HCl (X = H<sub>2</sub>) (III). In isolated guinea pig heart preps. 10<sup>-5</sup> M III increased heart contractile strength 127% and reduced heart rate 17%. Tablets were prepared each containing III 25.0, cornstarch 57.0, lactose 48.0, polyvinylpyrrolidone 4.0, and Mg stearate 1.0 mg.

IT 116578-58-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as inotropic intermediate)

RN 116578-58-6 CAPLUS

CN 4-Isoquinolineacetamide, N-[3-(3,4-dihydro-6,7-dimethoxy-1-oxo-2(1H)-isoquinolinyl)propyl]-6,7-dimethoxy-N-methyl- (9CI) (CA INDEX NAME)



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